AN ACCURACY STUDY OF CENTRAL FINITE DIFFERENCE METHODS

IN SECOND ORDER BOUNDARY VALUE PROBLEMS

By

Nancy Jane Cyrus

Thesis submitted to the Graduate Faculty of the

Virginia Polytechnic Institute

in candidacy for the degree of

MASTER OF SCIENCE

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MATHEMATICS

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ABSTRACT

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An accuracy study is made of central finite difference methods for solving boundary value problems which are governed by second order differential equations with variable coefficients leading to odd order derivatives. Three methods are studied through applications to selected problems. Definitive expressions for the error in each method are obtained by using Taylor series to derive the differential equations which exactly represent the finite difference approximations. The resulting differential equations are accurately solved by a perturbation technique which yields the error directly. A half station method, which corresponds to making finite difference approximations before expanding derivatives of function products in the differential equations, was found superior to two whole station methods which correspond to expanding such products first.

Author

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IV. INTRODUCTION

In the mathematical analysis of many physical boundary value problems, such as beams, plates and shells in structural analysis, the governing differential equations are often solved by approximating the derivatives by finite differences and solving the resulting system of algebraic equations on a digital computer. In the analysis of complicated structures the number of simultaneous equations resulting from finite differences may be large enough to exceed the capacity of the computer or to introduce round-off error in obtaining a numerical solution. For such problems, it is important to keep the number of algebraic equations at a minimum and the accuracy of the difference procedure can be a critical item in obtaining meaningful results. In reference 2, for example, it was found that accurate answers for the stresses in a shell structure could not be obtained by using certain finite difference approximations unless the mesh spacing was smaller than machine capacity permitted.

The most popular difference approximations used in boundary value problems are the central difference approximations which are given in textbooks on numerical methods. There are alternate formulations of central differences which can be used when odd order derivatives occur in the differential equation and these alternate formulations give different answers. It was shown in reference 14 that for a circular plate symmetrically loaded, approximating the differential equation by central differences led to a nonsymmetric matrix instead of the expected symmetric matrix. Furthermore, the answers in no way

resembled the known solutions to the problem and the central difference equation was singular at the center of the plate, a physically real point in the problem.

The purpose of this paper is to investigate the accuracy of the three alternate forms of central finite difference approximations as applied to boundary value problems. An approach for studying the accuracy of finite difference methods is presented and utilized. The study is confined to linear second order boundary value problems of a certain type but the approach and conclusions are applicable to a wide class of boundary value problems.

V. General Discussion of Error

Types of Error

The use of finite difference approximation formulas to obtain numerical solutions to differential equations leads to errors which can be classified as three types: (1) round-off error, (2) inherited error, and (3) truncation or discretization error. Round-off error is a calculation error resulting from using a finite number specified by n correct digits to approximate a number which requires more than n digits for its exact specification. Round-off error increases with the number of calculations required to get an answer. The inherited error is the contribution to the error due to the total error at a preceding step. This may result from using a step-by-step procedure in which each step uses the result from the previous step.

Truncation error, or discretization error as it is sometimes called, comes from approximating or replacing the continuous problem by a discrete model. Discretization error is decreased by using smaller increments; but as increment size decreases, the number of steps taken increases, calculations increase, and the danger that round-off error will build up to substantial proportions grows. In any problem that is short enough to permit hand computation, it is usually possible to carry enough places so that round-off error can be neglected. In extended computations using computing machines round-off error can be serious.

All three types of error can occur when a boundary value differential equation is solved by reducing it to an initial value problem

and then solving it by one of the step-by-step procedures for initial value problems (ref. 10). If a boundary value problem is solved by replacing the differential equation by central difference equations, taking into account the boundary conditions at both ends, and thus obtaining a set of simultaneous algebraic equations, inherited error does not exist as a separate entity. For such problems round-off and truncation error are the only separable effects. Round-off error, while it can be important in a practical problem utilizing large numbers of simultaneous equations, is not considered here.

Literature Survey

Numerous studies have been reported in the literature dealing with errors resulting from the use of numerical methods to approximate the solutions to linear and nonlinear ordinary and partial differential equations governing boundary value problems. A common way to solve a boundary value problem approximately is to reformulate the problem as an initial value problem and solve it using numerical integration. Consequently most of the error studies in the literature deal with initial value problems. However, some comments on a few important papers and books which do treat errors in boundary value problems are given here.

Collatz (ref. 3) gives methods for solving boundary value problems directly and for obtaining estimates of the discretization error. This is accomplished by first expanding the difference equations in Taylor series, then deriving a system of equations for

the errors, estimating higher order derivatives in some way and then solving the system of error equations to obtain error bounds.

In Modern Computational Methods, reference 13, a difference correction is added to the central difference approximations for the derivatives. A first approximation solution to the resulting system is obtained by neglecting the difference correction and solving the resulting algebraic equations. Then considering the difference correction a successive correction method is used to obtain corrections to the first approximation solution. The process is continued until there is no change in the numerical solution.

Many methods of error analysis of boundary value problems in partial differential equations are also applicable to ordinary differential equations. In the classic method developed by Gerschgorin (ref. 6), the discretization error is estimated by the use of a special method which he calls the majorant method. This method is also discussed by Collatz (ref. 3) and Forsythe and Wasow (ref. 5). Roudebush (ref. 15) uses an error analysis of the Gerschgorin type to show that the order of discretization error in ordinary differential equations and parabolic and elliptic partial differential equations is unaffected by a finite number of discontinuities in the coefficients of the differential equation. In this paper he derives some higher order finite difference approximations and shows that when these approximations are used the order of the discretization error is improved.

Bramble and Hubbard (ref. 1) have included the work of Gerschgorin (ref. 6) and Collatz (ref. 3) as special cases in their theorem for estimating error in the Dirchlet problem for elliptic equations.

In many studies of physical problems approximate methods are judged with the knowledge of what the correct solution should be. In Chuang and Veletsos (ref. 2), for example, two finite difference methods are used to obtain approximate solutions to the partial differential equations governing the deformation of cylindrical shell structures. One method gives results which are unacceptable, even as design data, while the other method gives a satisfactory solution.

Round-off error resulting from the solution of tridiagonal matrices, which result from the use of central difference methods in some boundary value problems, is not the concern in the present paper but has been treated to some extent in the literature. Von Neumann and Goldstine (ref. 19) establish an error bounds for which solutions by the elimination method is valid. Turing (ref. 18) discusses different matrix methods and gives round-off errors for the Jordan, Gauss and Choleski methods. Wilkinson (ref. 20) also gives estimates of round-off error in matrix solutions, while Lowan (ref. 11) deals specifically with tridiagonal matrices.

VI. DEVELOPMENT OF FINITE DIFFERENCE OPERATORS

Finite difference operators can be obtained by several methods. Three common procedures are given and used to derive the difference approximations investigated in the study.

Polynomial Approximation

One method of obtaining approximate values for the derivatives of a function which is known at a discrete number of points consists of fitting the given points with an appropriate polynomial, whose derivatives are then obtained. Referring to figure 1 the problem is to find the derivatives of the function which passes through the given points $(x_o, y_o), (x_1, y_1) \cdots (x_n, y_n)$. Values of the function are known at these points or stations.

Lagrange's interpolation formula can be specialized to fit a polynomial through a certain number of points. Let there be given values of the ordinates $y_o, y_1 \cdots y_n$ of the function $y = f(x)$ at the $(n + 1)$ points $x_o, x_1, \cdots x_n$. The polynomial of the nth degree through these points may be written in the form

$$y = P(x) = \frac{(x - x_1)(x - x_2) \cdots \cdots (x - x_n)}{(x_o - x_1)(x_o - x_2) \cdots \cdots (x_o - x_n)} f(x_o)$$

$$+ \frac{(x - x_o)(x - x_2) \cdots \cdots (x - x_n)}{(x_1 - x_o)(x_1 - x_2) \cdots \cdots (x_1 - x_n)} f(x_1)$$

$$+ \cdots \cdots \cdots \cdots \cdots$$

$$+ \frac{(x - x_o) \cdot \cdot \cdot (x - x_{i-1})(x - x_{i+1}) + \cdot \cdot \cdot (x - x_n)}{(x_i - x_o) \cdot \cdot \cdot (x_i - x_{i-1})(x_i - x_{i+1}) \cdot \cdot \cdot (x_i - x_n)} f(x_i)$$

$$+ \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot$$

$$+ \frac{(x - x_o)(x - x_1) \cdot \cdot \cdot (x - x_{n-1})}{(x_n - x_o)(x_n - x_1) \cdot \cdot \cdot \cdot (x_n - x_{n-1})} f(x_n) \tag{6.1}$$

The equation for a polynomial passing through three points separated by equal increments h and with the origin at $x = x_o$ is obtained from equation (6.1)

$$y(x) = y_o + \frac{x}{2h}\left(-3y_o + 4y_1 - y_2\right) + \frac{x^2}{2h^2}\left(y_o - 2y_1 + y_2\right) \tag{6.2}$$

The first derivative of the function is

$$y'(x) = \frac{1}{2h}\left(-3y_o + 4y_1 - y_2\right) + \frac{x}{h^2}\left(y_o - 2y_1 + y_2\right) \tag{6.3}$$

The slope at each of the points x_i is obtained by substituting $x = x_o = 0$, $x = x_1 = h$, $x = x_2 = 2h$ in equation (6.3). The second derivative of the curve $y(x)$ is

$$y''(x) = \frac{1}{h^2}\left(y_o - 2y_1 + y_2\right) \qquad (6.4)$$

which is constant because $y(x)$ is a second degree curve.

Polynomials passing through four points and five points can be obtained in a similar fashion and their derivatives evaluated at each point to obtain various difference patterns. Thus, numerous choices are available when selecting a difference pattern. Which pattern is best depends to a large extent on the equation to be solved and its boundary conditions. However, one set of central difference operators is usually suggested in textbooks (refs. 4, 10, and 16), widely used in the literature (refs. 2, 12, and 14), and generally accepted as preferred because of simplicity, ease with which boundary conditions are handled, and consistency of order of error. These are given in equations (6.5) to (6.8)

$$y'\left(x_i\right) = \frac{1}{2h}\left(-y_{i-1} + y_{i+1}\right) \qquad (6.5)$$

$$y''\left(x_i\right) = \frac{1}{h^2}\left(y_{i-1} - 2y_i + y_{i+1}\right) \qquad (6.6)$$

$$y^{iii}\left(x_i\right) = \frac{1}{2h^3}\left(-y_{i-2} + 2y_{i-1} + 0 - 2y_{i+1} + y_{i+2}\right) \qquad (6.7)$$

$$y^{iv}\left(x_i\right) = \frac{1}{h^4}\left(y_{i-2} - 4y_{i-1} + 6y_i - 4y_{i+1} + y_{i+2}\right) \qquad (6.8)$$

The simplicity of the selected operators equations (6.5) to (6.8) compared with writing at each station equations (6.3), (6.4), or those obtained from polynomials through four or five points (see ref. 16), to obtain the various difference operators is obvious. The order of the truncation error for each operator may be obtained by expanding the function $y(x_i)$ about the point x_i in Taylor series as given below

$$y(x_i + ah) = y(x_i) + ah\, y'(x_i) + \frac{(ah)^2}{2!} y''(x_i) + \cdots + \frac{(ah)^n}{n!} y^n(x_i)$$

$$= \sum_{n=0}^{\infty} \frac{(ah)^n}{n!} y^n(x_i) \qquad (6.9)$$

where y^n stands for the derivative $\frac{d^n y}{dx^n}$, a is any real number and h is the increment of the interval. For example, equation (6.5) which is (6.3) evaluated at the center, can be expanded as follows

$$-y_{i-1} = -y_i + hy_i' - \frac{h^2}{2} y_i'' + \frac{h^3}{6} y_i^{iii} - \frac{h^4}{24} y_i^{iv} + \frac{h^5}{120} y_i^v + \cdots$$

$$y_{i+1} = y_i + hy_i' + \frac{h^2}{2} y_i'' + \frac{h^3}{6} y_i^{iii} + \frac{h^4}{24} y_i^{iv} + \frac{h^5}{120} y_i^v + \cdots$$

$$-y_{i-1} + y_{i+1} = 0 + 2hy_i' + 0 + \frac{2h^3}{6} y_i^{iii} + 0 + \frac{2h^5}{120} y_i^v + \cdots$$

$$\frac{1}{2h}\left(-y_{i-1} + y_{i+1}\right) = y_i' + \frac{h^2}{6} y_i^{iii} + \frac{h^4}{120} y_i^v + \cdots$$

The truncation error is of order h^2 and is

$$\frac{h^2}{6} y_i^{iii} + \frac{h^4}{120} y_i^{v} + \cdots \tag{6.10}$$

For the first difference, equation (6.3) evaluated at the left end point leads to

$$\frac{1}{2h}\left(-3y_i + 4y_{i+1} + y_{i+2}\right)$$

and the truncation error is

$$-\frac{h^2}{3} y_i^{iii} - \frac{h^3}{4} y_i^{iv} - \frac{7}{60} h^4 y_i^{v} + \cdots \tag{6.11}$$

The second difference, equation (6.4) evaluated at the center point, is equation (6.6). It yields a truncation error of

$$\frac{h^2}{12} y_i^{iv} + \frac{h^4}{360} y_i^{vi} + \cdots \tag{6.12}$$

The second difference, equation (6.4) evaluated at the left end point gives the truncation error

$$h y_i^{iii} + \frac{7h^2}{12} y_i^{iv} + h^3 y_i^{v} + \cdots \tag{6.13}$$

Note from equations (6.10) to (6.13) that while the error for both first difference operators is of order h^2, the error for the second difference operator about an end point is of order h, and

about the center point, of order h^2. Generally, difference patterns with the same order of error are used for more consistent results. For example, one of the first difference patterns (error of order h^2), is not mixed with the second difference pattern at the end point (error of order h). When inconsistent order of error terms are used, the answers tend toward the more inaccurate terms (ref. 16).

Difference Operations

A second method for obtaining the various finite difference operators is differencing differences. The inverted delta, ∇, designates backward differences, the normal delta, Δ, forward differences and the lower case delta, δ, central differences. Suppose the values $f_i = f(x_i)$ of a function $f(x)$ are known at $(n + 1)$ equidistant points $x_i = a + ih$ where $i = 0, 1, 2, --- n$ (sometimes i is nonintegral). On the interval (a, b) h is the increment $\frac{b-a}{n}$ and is taken to be positive. For any function $f(x)$ the difference operators Δ, ∇, δ are defined for increment h as follows

$$\Delta f_i = f_{i+1} - f_i \tag{6.14}$$

$$\nabla f_i = f_i - f_{i-1} \tag{6.15}$$

$$\delta f_i = f_{i+\frac{1}{2}} - f_{i-\frac{1}{2}} \tag{6.16}$$

The differences in equations (6.14) to (6.15) may be extended to higher order differences by taking the difference of the difference; for example

$$\Delta^2 f_i = \Delta(\Delta f_i) = \Delta(f_{i+1} - f_i) = f_{i+2} - 2f_{i+1} + f_i \tag{6.17}$$

In general

$$\Delta^p f_i = \Delta(\Delta^{p-1} f_i) \qquad \nabla^p f_i = \nabla(\nabla^{p-1} f_i) \qquad \delta^p = \delta(\delta^{p-1} f_i)$$

$$p = 1, 2 \cdots \tag{6.18}$$

for $p = 0$

$$\Delta^0 f_i = \nabla^0 f_i = \delta^0 f_i = f_i \tag{6.19}$$

Given in equations (6.20a) to (6.22e) are the finite difference operators that approximate the various order derivatives (including zero order). Also included are the operators expanded in Taylor series to obtain truncation error terms.

Forward Differences

$$
\begin{array}{lllllll@{\quad}l}
\text{Derivative} & \multicolumn{5}{l}{\text{Finite difference pattern}} & \text{Taylor series expansion} & \\
 & i & i+1 & i+2 & i+3 & i+4 & & \\
y_i \approx 1 & (\;1 & & & &) & = y_i + 0 & \text{(a)} \\
y_i' \approx \frac{1}{h} & (-1 & 1 & & &) & = y_i' + \frac{h}{2} y_i'' + \frac{h^2}{6} y_i^{iii} + \cdots & \text{(b)} \\
y_i'' \approx \frac{1}{h^2} & (\;1 & -2 & 1 & &) & = y_i'' + h\, y_i^{iii} + \frac{7h^2}{12} y_i^{iv} + \cdots & \text{(c)} \\
y_i^{iii} \approx \frac{1}{h^3} & (-1 & 3 & -3 & 1 &) & = y_i^{iii} + \frac{3}{2} h\, y_i^{iv} + \frac{5}{4} h^2 y_i^{v} + \cdots & \text{(d)} \\
y_i^{iv} \approx \frac{1}{h^4} & (\;1 & -4 & 6 & -4 & 1\;) & = y_i^{iv} + 2\, h\, y_i^{v} + \frac{13}{6} h^2 y^{vi} + \cdots & \text{(e)}
\end{array}
\tag{6.20}
$$

Backward Differences

Derivative		Finite difference pattern					Taylor series expansion	
		i-4	i-3	i-2	i-1	i		
y_i	≈ 1 (					1)	$= y_i + 0$	(a)
y_i'	$\approx \frac{1}{h}$ (				1	1)	$= y_i' - \frac{h}{2} y_i'' + \frac{h^2}{6} y^{iii} + \cdots$	(b)
y_i''	$\approx \frac{1}{h^2}$ (			1	-2	1)	$= y_i'' - h\, y_i^{iii} + \frac{7h^2}{12} y^{iv} + \cdots$	(c)
y_i^{iii}	$\approx \frac{1}{h^3}$ (		-1	3	-3	1)	$= y_i^{iii} - \frac{3}{2} y_i^{iv} + \frac{5h^2}{4} y^{v} + \cdots$	(d)
y_i^{iv}	$\approx \frac{1}{h^4}$ (	1	-4	6	-4	1)	$= y_i^{iv} - 2\, h\, y^{v} - \frac{13}{6} h^2 y^{vi} + \cdots$	(e)

(6.21)

Central Differences

Derivative		i-2	$i-\frac{3}{2}$	i-1	$i-\frac{1}{2}$	i	$i+\frac{1}{2}$	i+1	$i+\frac{3}{2}$	i+2	Taylor series expansion	
y_i	≈ 1 (					1				)	$= y_i + 0$	(a)
y_i'	$\approx \frac{1}{h}$ (				-1		1			)	$= y_i' + 0h\, y_i'' + \frac{1}{24} h^2 y_i^{iii} + \cdot$	(b)
y_i''	$\approx \frac{1}{h^2}$ (			1		-2		1		)	$= y_i'' + 0h\, y_i^{iii} + \frac{1}{12} h^2 y_i^{iv} + \cdot$	(c)
y_i^{iii}	$\approx \frac{1}{h^3}$ (		-1		3		-3		1	)	$= y_i^{iii} + 0h\, y^{iv} + \frac{1}{8} h^2 y_i^{v} + \cdot \cdot$	(d)
y_i^{iv}	$\approx \frac{1}{h^4}$ (	1		-4		6		-4		1)	$= y_i^{iv} + 0h\, y^{v} + \frac{1}{6} h^2 y_i^{vi} + \cdot \cdot$	(e)

(6.22)

Forward and backward differences give unilateral expressions for the derivatives of a function $y(x_i)$, which in their simplest form have errors of order h. Central differences, involving pivotal points or stations symmetrically located with respect to x_i, are particularly useful in the solution of boundary value problems, reference 3. Note that the order of error for the central difference operators is h^2. Generally, as h approaches zero the central differences approach the exact value faster than forward or backward differences.

The central difference operators (6.22a) to (6.22e) are defined at half stations for odd derivatives. These operators are regular and consistent and may be used successfully in boundary value problems. They will be referred to as "half station" operators.

The linear second order differential equation in the form

$$L(y) = a_o(x)y'' + a_1(x)y' + a_2(x)y = b(x) \qquad (6.23)$$

cannot be approximated by the half station operators because the approximation for second derivative introduces unknowns y_{i-1}, y_i, y_{i+1} and the approximation for first derivative introduces unknowns $y_{i-\frac{1}{2}}$, $y_{i+\frac{1}{2}}$. This gives too many unknowns for the number of equations. However, equation (6.23) may be reduced to the form

$$L(y) = \left[f(x)y'\right]' + g(x)y = p(x) \qquad (6.24)$$

by multiplying by

$$\frac{e^{\int_{x_o}^{x} \frac{a_1(x)}{a_o(x)}dx}}{a_o(x)}$$

Then

$$f = e^{\int_{x_o}^{x} \frac{a_1}{a_o}dx} \qquad g = \frac{a_2\, e^{\int_{x_o}^{x} \frac{a_1}{a_o}dx}}{a_o} \qquad p = \frac{e^{\int_{x_o}^{x} \frac{a_1}{a_o}dx}\, b}{a_o}$$

Equation (6.34) can be solved by using half station operators.

Averaging Procedure

The central difference operators (6.5) to (6.8) which were obtained from Lagrange's interpolation formula, and which do not have half stations in the approximations for odd order derivatives, can be obtained by averaging difference operators. The first averaged or mean difference at i is obtained by taking the average of the first central difference at $i-\frac{1}{2}$ and $i+\frac{1}{2}$. The operation is symbolized by the operator μ called the averager. The first averaged difference is

$$\mu\delta\, y_i = \frac{1}{2}\left[\delta y_{i-\frac{1}{2}} + \delta y_{i+\frac{1}{2}}\right] = \frac{1}{2}\left[\frac{1}{h}\left(-y_{i-1} + y_i\right) + \frac{1}{h}\left(-y_i + y_{i+1}\right)\right]$$

$$= \frac{1}{2h}\left[-y_{i-1} + y_{i+1}\right] \qquad (6.25)$$

Similarly the next averaged difference is

$$\mu\delta^3 y_i = \frac{1}{2}\left[\delta^3 y_{i-\frac{1}{2}} + \delta^3 y_{i+\frac{1}{2}}\right] = \cdots = \frac{1}{2h^3}\left[-y_{i-2} + 2y_{i-1} - 2y_{i+1} + y_{i+2}\right]$$

Since the averaged central difference operators are defined only at integral points, that is at whole stations, they shall be referred to as "whole station" operators.

Expanding the whole station operators in a Taylor series to obtain the first two truncation error terms results in the following

Derivative		Finite difference pattern y_{i-2}	y_{i-1}	y_i	y_{i+1}	y_{i+2}	Taylor series expansion	
y_i	≈ 1	(		1		)	$= y_i + 0$	(a)
y_i'	$\approx \frac{1}{2h}$	(	-1	0	-1	)	$= y_i' + \frac{h^2}{6} y_i^{iii} + \cdots$	(b)
y_i''	$\approx \frac{1}{h^2}$	(	1	-2	1	)	$= y_i'' + \frac{h^2}{12} y_i^{iv} + \cdots$	(c)
y_i^{iii}	$\approx \frac{1}{2h^3}$	(-1	2	0	-2	1)	$= y_i^{iii} + \frac{h^2}{4} y_i^{v} + \cdots$	(d)
y_i^{iv}	$\approx \frac{1}{h^4}$	(1	-4	6	-4	1)	$= y_i^{iv} + \frac{h^2}{6} y_i^{vi} + \cdots$	(e)

(6.26)

This study is concerned with determining and comparing the accuracy of the two central difference methods both with order of error h^2, the half and whole station methods. Also a modified form

of the whole station method, in which all derivatives occurring in the given equation $L(y)$ are approximated, is considered.

VII. A Method for Determining the Accuracy of the Central Finite Difference Equations

To study the accuracy of the half station and whole station methods in second order boundary value problems, the simple problem

$$L(y) = -(fy')' + gy = p(x) \tag{7.1}$$

with boundary conditions

$$y(a) = y_a \qquad y(b) = y_b$$

on the interval (a,b) is considered.

With $h = \frac{b-a}{n}$ and $x_i = a + ih$ the finite difference method, applying operator equation (6.16) to equation (7.1), and noting that

$$-(fy')'_i = \frac{1}{h}\left[-(fy')_{i-\frac{1}{2}} + (fy')_{i+\frac{1}{2}}\right]$$

$$= -\frac{1}{h}\left[-f_{i-\frac{1}{2}}\frac{1}{h}\left(-y_{i-1} + y_i\right) + f_{i+\frac{1}{2}}\frac{1}{h}\left(-y_i + y_{i+1}\right)\right]$$

yields

1. Half Station Method

$$-\frac{1}{h^2}\left[f_{i-\frac{1}{2}}y_{i-1} - \left(f_{i-\frac{1}{2}} + f_{i+\frac{1}{2}}\right)y_i + f_{i+\frac{1}{2}}y_{i+1}\right] + g_iy_i - p_i = 0 \tag{7.2}$$

$$y_o = y_a \qquad y_n = y_b \qquad (i = 1, 2, \cdots n-1)$$

Using the expanded form of equation (7.1),

$$L(y) = -f'y'' - fy' + gy = p(x) \qquad (7.3)$$

and the operators in equations (6.5), (6.6), the difference equation for (7.1) takes the form

2a. Whole Station Method

$$-\frac{1}{h^2}\left[\left(f_i - \frac{hf'_i}{2}\right) y_{i-1} - 2f_i\, y_i + \left(f_i + \frac{hf'_i}{2}\right) y_{i+1}\right] + g_i y_i - p_i = 0$$

$$(7.4)$$

$$y_o = y_a \qquad y_n = y_b \qquad (i = 1, 2, \cdots n - 1)$$

The derivative f'_i in equation (7.4) can be evaluated exactly at the appropriate stations. Another method which can be considered is to approximate f'_i by equation (6.26b). The result is

2b. Modified Whole Station Method

$$-\frac{1}{h^2}\left[\left(f_i - \frac{-f_{i-1} + f_{i+1}}{4}\right) y_{i-1} - 2f_i\, y_i \right.$$

$$\left. + \left(f_i + \frac{-f_{i-1} + f_{i+1}}{4}\right) y_{i+1}\right] + g_i y_i - p_i = 0 \qquad (7.5)$$

$$y_o = y_a \qquad y_n = y_b \qquad (i = 1, 2, \cdots n - 1)$$

Note that the three sets of finite difference equations, (7.2), (7.4), and (7.5), lead to different coefficients for the simultaneous equations in terms of the same displacements y_i at the i^{th} station. With a few assumptions the existence and uniqueness of the solution of each of the sets of simultaneous equations is established from a theorem proved by Collatz and stated in appendix A.

If it is assumed that $f(x) > 0$ and $g(x) \geq 0$, the systems of equations (7.2) and (7.5) satisfy the conditions of Theorem A1 (in addition to the sign distribution, the weak row sum criterion is satisfied and the matrix of coefficients is irreducible); hence, a uniquely determined solution exists for each system for arbitrary boundary conditions and arbitrary values of p_1. For the set of equations (7.4) the additional assumption that for

$$f'(x) \neq 0, \ h < \left|\frac{2f}{f'}\right|$$

satisfies the conditions.

The usual approach in a finite difference accuracy study (ref. 12) is to carry out the numerical solution to a number of problems for which the exact solutions can be obtained and compare the resulting numerical answers with the exact answers. This procedure was carried out for a number of problems of the type of equation (7.1) and a table of relative error for a typical result is given in appendix B. Such a procedure has the liability that calculations must be redone each time the increment size, h, changes.

The root mean square of relative error for three different values of the increment h for problems solved is given in appendix B.

Conventional means for estimating the error bounds do not give a satisfactory means of comparison of the different methods since the error limits exceed the actual error in magnitude.

To obtain definitive expressions for error in each method, independent of increment h, first expand the finite difference recursion equations (7.2), (7.4), and (7.5) in a Taylor series expansion about the i^{th} point. For each method this leads to a differential equation of the form

$$L_o\left(y_i\right) - p_i + h^2 L_1\left(y_i\right) + h^4 L_2\left(y_i\right) + \cdots = 0 \qquad (7.6)$$

subject to the boundary conditions

$$y_i = y_a \qquad \text{at} \qquad x = a$$

$$y_i = y_b \qquad \text{at} \qquad x = b$$

The symbols L_0, L_1, and L_2 are linear differential operators given by

$$L_o\left(y_i\right) = -\left(f_i y_i'\right)' + g_i\, y_i \qquad (7.7)$$

and

1. Half Station Method

$$L_1(y_i) = -\left(\frac{f_i y_i^{iv}}{12} + \frac{f_i' y_i^{iii}}{6} + \frac{f_i'' y_i''}{8} + \frac{f_i^{iii} y_i'}{24}\right)$$

(7.8a)

$$L_2(y_i) = -\left(\frac{f_i y_i^{vi}}{360} + \frac{f_i' y_i^{v}}{120} + \frac{f_i'' y_i^{iv}}{96} + \frac{f_i^{iii} y_i^{iii}}{144} + \frac{f_i^{iv} y_i''}{384} + \frac{f_i^{v} y_i'}{1920}\right)$$

2a. Whole Station Method

$$L_1(y_i) = -\left(\frac{f_i y_i^{iv}}{12} + \frac{f_i' y_i^{iii}}{6}\right)$$

(7.8b)

$$L_2(y_i) = -\left(\frac{f_i y_i^{vi}}{360} + \frac{f_i' y_i^{v}}{120}\right)$$

2b. Modified Whole Station Method

$$L_1(y_i) = -\left(\frac{f_i y_i^{iv}}{12} + \frac{f_i' y_i^{iii}}{6} + \frac{f_i^{iii} y_i'}{6}\right)$$

(7.8c)

$$L_2(y_i) = -\left(\frac{f_i y_i^{vi}}{360} + \frac{f_i' y_i^{v}}{120} + \frac{f_i^{iii} y_i^{iii}}{120} + \frac{f_i^{v} y_i'}{36}\right)$$

Equation (7.6) and (7.7) together with (7.8a), (7.8b), or (7.8c) are clearly the differential equation which represent exactly the finite difference equations. As h approaches zero, equation (7.6) approaches equation (7.1). The solution to equation (7.6), satisfying

the appropriate boundary conditions, gives an analytical representation of the numerical finite difference answers. A closed form solution to equation (7.6) does not appear feasible since it contains an infinite number of terms. For a practical problem, however, if the length of the interval (a,b) is one unit, h is perhaps 0.1 or 0.01 or even smaller. This suggests that equation (7.6) can be solved with the use of perturbations with the parameter taken to be h^2.

Let the solution y_i to equation (7.6) be taken in the form

$$y_i = Y_o + h^2 Y_1 + \cdot \cdot \cdot \tag{7.9}$$

Substituting equation (7.9) into equation (7.6) leads to

$$L_o\left(Y_o\right) - p_i + h^2 \left[L_o\left(Y_1\right) + L_1\left(Y_o\right)\right] + \cdot \cdot \cdot = 0 \tag{7.10}$$

subject to

$$Y_o(a) + h^2 \left[Y_1(a)\right] + \cdot \cdot \cdot = 0$$

$$Y_o(b) + h^2 \left[Y_1(b)\right] + \cdot \cdot \cdot = 0$$

If each order of error term is solved in sequence, the following series of problems result.

(1) $L_o\left(Y_o\right) - p_i = 0 \qquad Y_o(a) = 0,\ Y_o(b) = 0 \qquad (7.11)$

(2) $L_o(Y_1) + L_1(Y_o) = 0 \qquad Y_1(a) = 0,\ Y_1(b) = 0 \qquad (7.12)$

(3) . . .

Note that since equation (7.1) is linear Y_o given by equation (7.11) is in fact the exact solution. From the form of y_i it is seen that Y_1 can be interpreted as the first order error term in the finite difference results. The magnitude of Y_1 is, therefore, a measure of the error in the finite difference results as compared to the exact answer to the problem. A comparison of the error terms Y_1 resulting from the different finite difference approximations indicates the relative accuracy of the different approximations.

While errors in the y_i are important, errors in numerically obtained derivatives should also be considered for a thorough error analysis. Therefore, results were obtained by using the finite difference answers for approximate second derivatives. The second difference operator was applied to the difference results followed by Taylor and perturbation series expansions to yield

$$y_i'' = \frac{1}{h^2}\left(y_{i-1} - 2y_i + y_{i+1}\right)$$

$$= Y_o'' + h^2 Y_1'' + \frac{h^2}{12}\left(Y_o^{iv} + h^2 Y_1^{iv} + \cdot \cdot \cdot\right) + \cdot \cdot \cdot$$

or

$$y_i'' = Y_o'' + h^2\left(Y_1'' + \frac{Y_o^{iv}}{12}\right) + \cdot \cdot \cdot \qquad (7.13)$$

VIII. Application of the Method to Particular Problems

Problems Studied

Using the method described in the previous section, the error term Y_1 in equation (7.9) and the second derivative error term $Y_1'' + \frac{Y_0^{iv}}{12}$ in equation (7.13) have been obtained for a series of problems for the half station and whole station approximations. Equation (7.1) has been solved with $g = 0$, $p = -1$ for the following values of $f(x)$

$$(1) \quad f(x) = \frac{1}{x^n} \qquad \text{for} \qquad 1 \leq n \leq 6 \quad 1 \leq x \leq 2 \tag{8.1}$$

subject to the boundary conditions

$$y(1) = 0$$

$$y(2) = 0$$

and

$$(2) \quad f(x) = 1 + x^n \qquad \text{for} \qquad 1 \leq n \leq 5 \quad 0 \leq x \leq 1 \tag{8.2}$$

subject to the boundary conditions

$$y(0) = 0$$

$$y(1) = 0$$

Physically these problems might correspond to the problem of lateral deflection of a string having a uniformly distributed lateral load and a variable tension force f(x).

For the case where f(x) is linear (corresponding to f(x) = 1, x, or 1 + x) the results for the half station and two whole station finite difference approximations are exactly the same. In fact for f(x) = 1, all three difference answers are the exact answer. For all other cases, however, the three difference methods lead to different results. It is useful to compare the results for the case $f(x) = \frac{1}{x^3}$ in detail as a typical example.

For $f(x) = \frac{1}{x^3}$ and $y(1) = y(2) = 0$

$$Y_o = -\frac{x^5}{5} + \frac{31}{75}x^4 - \frac{16}{75} \tag{8.3}$$

and

1. Half Station Method

$$Y_1 = -\frac{41}{1125}x^4 + \frac{x^3}{6} - \frac{31}{150}x^2 + \frac{86}{1125} \tag{8.4}$$

2a. Whole Station Method

$$Y_1 = -\frac{187}{450}x^4 + \frac{4}{3}x^3 - \frac{31}{30}x^2 + \frac{26}{225}$$

2b. Modified Whole Station Method

$$Y_1 = -\frac{103}{90}x^4 + \frac{14}{3}x^3 - \frac{31}{6}x^2 + \frac{74}{45} \tag{8.5}$$

A plot of the three error terms Y_1 over the unit interval is given in figure 2(b). The exact solution, Y_o is given in figure 2(a). The finite difference solution (7.9) can be obtained to the first two terms for any desired increment h from figures 2(a) and 2(b). Solutions were also obtained for the error terms for all of the remaining functions $f(x)$ noted previously; additional plots of results and the exact solution for the case $f(x) = 1 + x^3$, are shown in figures 3(a) and 3(b). Detailed plots of the remaining solutions are not shown because figures 2(b) and 3(b) serve to illustrate the character of the results; and overall measure of the relative errors in the two methods will be shown for all the solutions obtained.

The error terms for the second derivatives corresponding to the different methods and for the case $f(x) = \frac{1}{x^3}$ are as follows

1. Half Station Method

$$Y_1'' + \frac{Y_o^{iv}}{12} = -\frac{164}{375}x^2 - x + \frac{31}{75} \tag{8.6}$$

2a. Whole Station Method

$$Y_1'' + \frac{Y_o^{iv}}{12} = -\frac{374}{75}x^2 + 6x - \frac{31}{25} \tag{8.7}$$

2b. Modified Whole Station Method

$$Y_1'' + \frac{Y_o^{iv}}{12} = -\frac{206}{15}x^2 + 26x - \frac{713}{75} \tag{8.8}$$

A plot of the error in the second derivative for each of the methods is given in figure 2(d) for this case and in figure 3(d) for the case $f(x) = 1 + x^3$. The exact solutions Y''_o are given in figures 2(c) and 3(c). Again the first two terms of the finite difference solution (7.13) can be obtained from these plots for the desired increment h. Results for the remaining functions will be shown later.

Numerical calculations were also carried out for the deflections and the second derivatives for the problems cited to determine if the analytical errors adequately represented the numerical errors. The data are not included here; however, for h less than about 0.1 all numerical errors agree with analytical errors to within one percent.

Relative Errors of the Half and Whole Stations Methods

While results such as those given in figures 2 and 3 are usually sufficient to identify which of the methods is superior for a given problem, identification of the superior method for specific results is sometimes difficult. A quantitative measure of the relative accuracy of the methods can be made by examining the root mean square values of the errors for the entire solution, that is

$$\overline{Y}_1 = \sqrt{\int_{x_o}^{x_o+1} Y_1^2 \, dx}$$

for the error in deflection and

$$\overline{Y}_1'' = \sqrt{\int_{x_o}^{x_o+1} \left(Y_1'' + \frac{Y_o^{iv}}{12} \right)^2 dx}$$

for the error in second derivative, where the integration is over the unit length from a to b. Thus, to assess quantitatively the relative merits of the half station and whole station methods for the various problems solved, the ratios

$$\frac{\overline{Y}_{1,half}}{\overline{Y}_{1,whole}}$$

$$\frac{\overline{Y}''_{1,half}}{\overline{Y}''_{1,\ whole}}$$

have been calculated for each problem. The results are shown in figure 4. Ratios for the modified form of the whole station method compared with the half station method are given in figure 5.

Discussion of Results

The results given in figures 4 and 5 show that for the problems studied the error in the deflection resulting from use of the half station method is less than the error resulting from the use of the whole station method. The investigation of the accuracy of the second derivative approximations gives the same result in general.

The difference between the two methods is generally less in calculating the second derivatives of deflections than in calculating the deflections themselves; moreover, differences in the comparative error from problem to problem are noticeably less with the second derivatives than with the deflections.

It should be noted that the analytical representation of errors shows clearly the danger of using numerical data at a single station or a few points to characterize the error in a problem. A typical case is shown in figure 2(d) for $f(x) = \frac{1}{x^3}$. If comparisons are made of the second derivatives near the end $x = 1$, the whole station method appears much more accurate than the half station method; however, figure 4(b) shows clearly that the average error with the whole station method is more than twice as great.

Reasons for the superiority of the half station method are not altogether clear, but may include the symmetry of the matrix of coefficients in this method. By contrast, the matrix of coefficients associated with whole stations is not symmetric. Matrix symmetry can be of great value for many numerical procedures associated with eigenvalue routines and simultaneous equation solving routines and, in some cases, is required for an efficient numerical solution of a large order system.

IX. CONCLUSION

A procedure was developed to determine an analytical expression for the discretization error in a finite difference solution to allow a direct comparison of methods which was independent of the increment, or mesh size. Using this procedure, a comparison was made of the accuracy of two different finite difference methods for solving linear second order boundary value problems.

The methods investigated were a "half station" method which corresponds to making the finite difference approximation before expanding the derivatives of function products and a "whole station" method which corresponds to expanding such products before making the approximations. Both of these methods are currently in use. Also investigated was an alternate form of the whole station method in which known derivatives are approximated rather than evaluated exactly. It was found that, for the same number of stations, the average error in calculated deflection resulting from use of half station difference approximations was always less than the error which resulted from the use of the whole station difference approximations. In some cases this error is reduced by an order of magnitude. It was also found that the alternate form of the whole station method gave the same or better results than the usual whole station approximation. The investigation of the accuracy of second derivatives gave similar results in general.

X. BIBLIOGRAPHY OF SOME PUBLICATIONS ON NUMERICAL METHODS

Numerous publications concerned with the numerical solution of differential equations and the accuracy of these solutions are found in the literature. Those publications that are useful in the present study of the accuracy of central finite difference methods for approximating the solution of boundary value problems in ordinary differential equations are listed as references in this paper. In addition a number of publications which are concerned with the numerical solution of initial value problems, or problems which can be changed to this type, and the numerical solution of partial differential equations are given in the bibliography.

The bibliography is arranged in five sections. Included in the first section are publications in which the theory of one or more of the different methods for obtaining numerical solutions is discussed. In some of these articles, discussions on stability, convergence and accuracy are included. The second section includes publications in which the emphasis is placed on error estimates and error bounds. The third section contains publications which report on the methods used to obtain approximate solutions of particular physical problems. In the fourth section are books on methods of numerical analysis. The last section contains some extensive bibliographies which cover the different areas of numerical analysis.

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XIII. VITA

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Nancy Jane Cyrus

XIV. APPENDIX A

The following theorem is proved by Collatz (ref. 3, page 44).

Theorem A 1. If the coefficients a_{jk} of an $n \times n$ matrix A satisfy the conditions

1. Sign distribution $a_{jj} > 0$, $a_{jk} \leq 0$ for $j \neq k$

2a. The weak row-sum criterion

$$\sum_{k=1}^{n} a_{jk} \begin{cases} \geq 0 & \text{for } j = 1, 2 \cdots n \\ > 0 & \text{for at least one } j = j_o \end{cases}$$

and 2b. Matrix A is irreducible or instead of 2a and b the stronger condition

2c. Ordinary row sum criterion

$$\sum_{k=1}^{n} a_{jk} > 0 \qquad \text{for} \qquad j = 1, \ldots n,$$

then A is monotonic and det $A \neq 0$. Thus a unique solution to A exists.

XV. APPENDIX B

The problems named in equations (8.1) and (8.2) were solved exactly and numerically by the half station, whole station, and modified whole station methods with the increment h equal to 0.25, 0.125, and 0.0625. The relative error R was calculated for each method. An example of the table of exact and approximate solutions and the relative errors at several points is given in table I for the problem $-((1 + x^3)y')' = 1$. Rather than include similar tables for each problem, the root mean square of the relative error given by

$$\sqrt{R_1^2 + R_2^2 + \cdot \cdot \cdot + R_n^2}$$

was found for each method. The root mean square errors for each method for each increment h are given in table II. After examining tables I and II it is seen that it is sometimes difficult to determine which method is best for the desired increment h.

TABLE I

EXACT SOLUTION, APPROXIMATE SOLUTIONS AND RELATIVE ERRORS OF APPROXIMATE SOLUTIONS TO THE EQUATION $-((1 + x^3)\, y')' = 1$ WITH THE BOUNDARY CONDITIONS $y(0) = y(1) = 0$

x	Exact solution	Half station approximation	Whole station approximation	Modified whole station approximation	% Error half	% Error whole	% Error modified whole
0.2500	0.08026543	0.08105831	0.08220624	0.08255914	0.99	2.42	2.86
0.5000	0.09778593	0.09883737	0.10055356	0.10048789	1.08	2.83	2.76
0.7500	0.06311073	0.06364571	0.06479616	0.06449213	0.85	2.67	2.19
0.1250	0.04804369	0.04814215	0.04828157	0.04836306	0.20	0.50	0.66
0.2500	0.08026543	0.08045903	0.08073254	0.08081650	0.24	0.58	0.69
0.3750	0.09660985	0.09686135	0.09723406	0.09727394	0.26	0.65	0.69
0.5000	0.09778593	0.09804143	0.09844953	0.09843154	0.26	0.68	0.66
0.6250	0.08565525	0.08586286	0.08623443	0.08617246	0.24	0.68	0.60
0.7500	0.06311073	0.06324233	0.06351694	0.06344181	0.21	0.64	0.52
0.8750	0.03350850	0.03356466	0.03370672	0.03365383	0.17	0.59	0.43
0.0625	0.02598403	0.02599588	0.02601276	0.02602580	0.05	0.11	0.16
0.1250	0.04804369	0.04806812	0.04810261	0.04812281	0.05	0.12	0.16
0.1875	0.06614644	0.06618320	0.06623503	0.06625746	0.06	0.13	0.17
0.2500	0.08026543	0.08031322	0.08038109	0.08040184	0.06	0.14	0.17
0.3125	0.09040258	0.09045918	0.09054076	0.09055695	0.06	0.15	0.17
0.3750	0.09660985	0.09667225	0.09676432	0.09677411	0.06	0.16	0.17
0.4375	0.09900592	0.09907062	0.09916924	0.09917180	0.07	0.16	0.17
0.5000	0.09778593	0.09784934	0.09795012	0.09794555	0.06	0.17	0.16
0.5625	0.09322215	0.09328098	0.09337940	0.09336861	0.06	0.17	0.16
0.6250	0.08565525	0.08570683	0.08579861	0.08578314	0.06	0.17	0.15
0.6875	0.07547746	0.07552005	0.07560139	0.07558320	0.06	0.16	0.14
0.7500	0.06311073	0.06314349	0.06321136	0.06319264	0.05	0.16	0.13
0.8125	0.04898331	0.04900631	0.04905850	0.04904148	0.05	0.15	0.12
0.8750	0.03350850	0.03352252	0.03355766	0.03354449	0.04	0.15	0.11
0.9375	0.01706786	0.01707413	0.01709166	0.01708425	0.04	0.14	0.10

TABLE II

ROOT MEAN SQUARES OF THE RELATIVE ERRORS OBTAINED IN APPROXIMATING THE EQUATION $-(f(x)y')' = 1$

$f(x) = \frac{1}{x}$

Size of increment, h	1/4	1/8	1/16
% error using half station method	.42	.16	.06
% error using whole station method	1.69	.65	.24
% error using modified whole station method	1.29	.46	.16

$f(x) = \frac{1}{x^2}$

Size of increment, h	1/4	1/8	1/16
% error using half station method	.31	.12	.04
% error using whole station method	3.82	1.43	.52
% error using modified whole station method	.74	.74	.28

$f(x) = \frac{1}{x^3}$

Size of increment, h	1/4	1/8	1/16
% error using half station method	.39	.16	.06
% error using whole station method	5.91	2.13	.77
% error using modified whole station method	3.93	1.93	.78

$f(x) = \frac{1}{x^4}$

Size of increment, h	1/4	1/8	1/16
% error using half station method	1.62	.64	.24
% error using whole station method	7.43	2.57	.92
% error using modified whole station method	12.00	5.52	2.17

$f(x) = \frac{1}{x^5}$

Size of increment, h	1/4	1/8	1/16
% error using half station method	3.40	1.34	.50
% error using whole station method	8.15	2.79	1.00
% error using modified whole station method	28.22	12.10	4.69

$f(x) = \frac{1}{x^6}$

Size of increment, h	1/4	1/8	1/16
% error using half station method	5.67	2.24	.83
% error using whole station method	9.01	3.38	1.28
% error using modified whole station method	52.40	22.11	8.55

$f(x) = 1 + x$

Size of increment, h	1/4	1/8	1/16
% error using half station method	.90	.35	.14
% error using whole station method	.90	.35	.14
% error using modified whole station method	.90	.35	.14

$f(x) = 1 + x^2$

Size of increment, h	1/4	1/8	1/16
% error using half station method	1.16	.45	.17
% error using whole station method	3.25	1.23	.45
% error using modified whole station method	3.25	1.23	.45

$f(x) = 1 + x^3$

Size of increment, h	1/4	1/8	1/16
% error using half station method	1.69	.54	.22
% error using whole station method	4.58	1.64	.58
% error using modified whole station method	4.54	1.62	.59

TABLE II.- Continued

$f(x) = 1 + x^4$

Size of increment, h	1/4	1/8	1/16
% error using half station method	2.18	.78	.28
% error using whole station method	5.79	2.08	.75
% error using modified whole station method	4.14	1.35	.47

$f(x) = 1 + x^5$

Size of increment, h	1/4	1/8	1/16
% error using half station method	2.72	.97	.34
% error using whole station method	7.12	2.56	.92
% error using modified whole station method	3.05	.88	.31

TABLE II.- Concluded

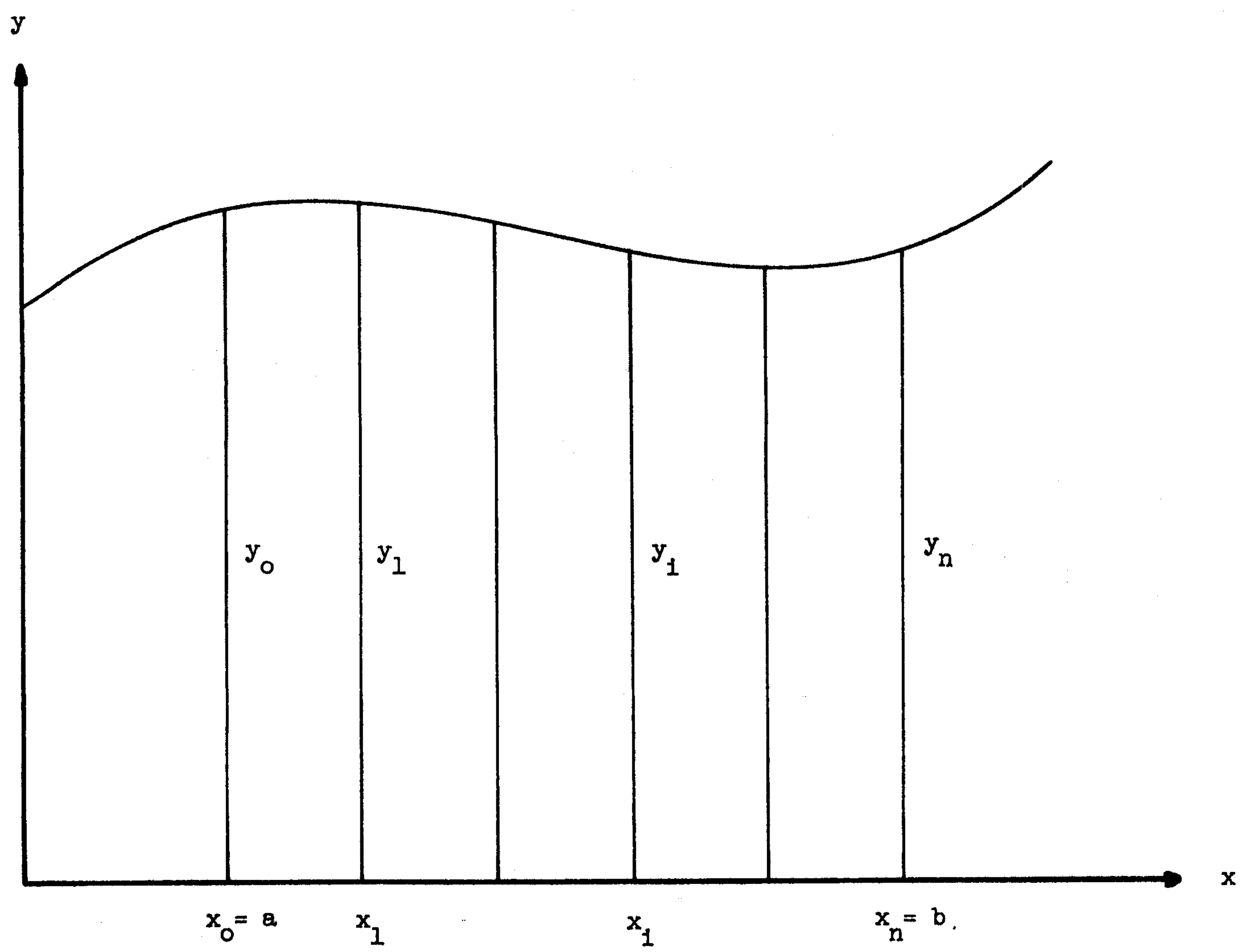
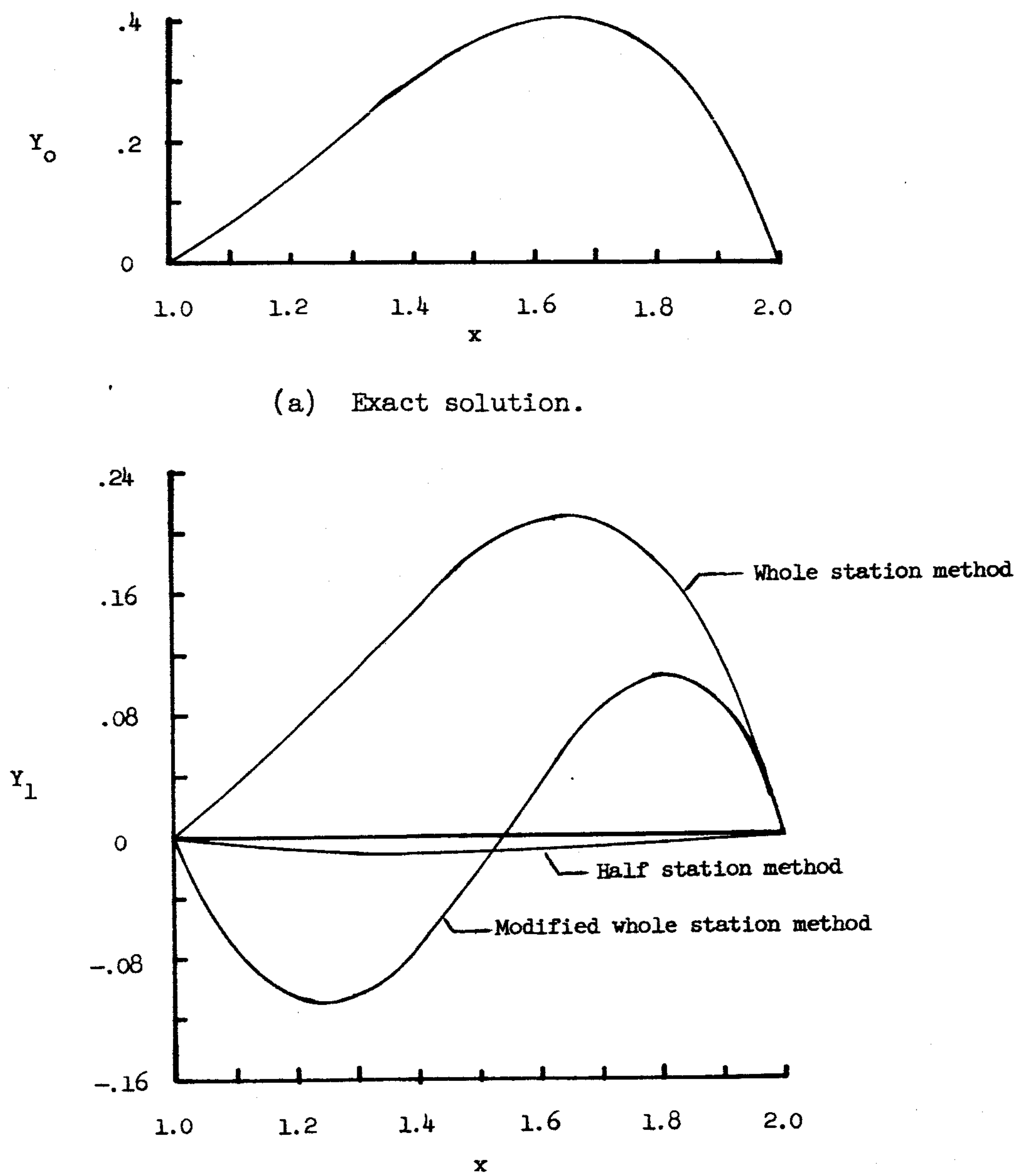


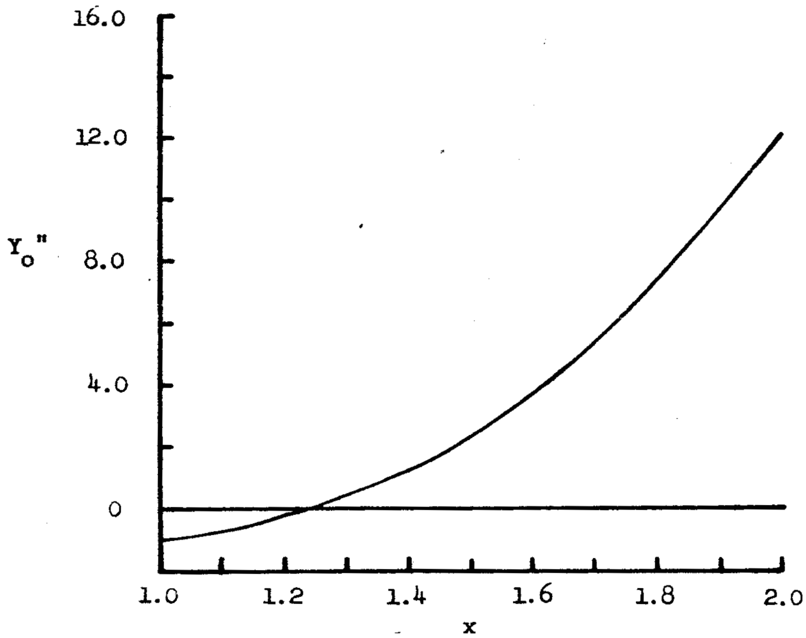
Figure 1.- Function $y = f(x)$.



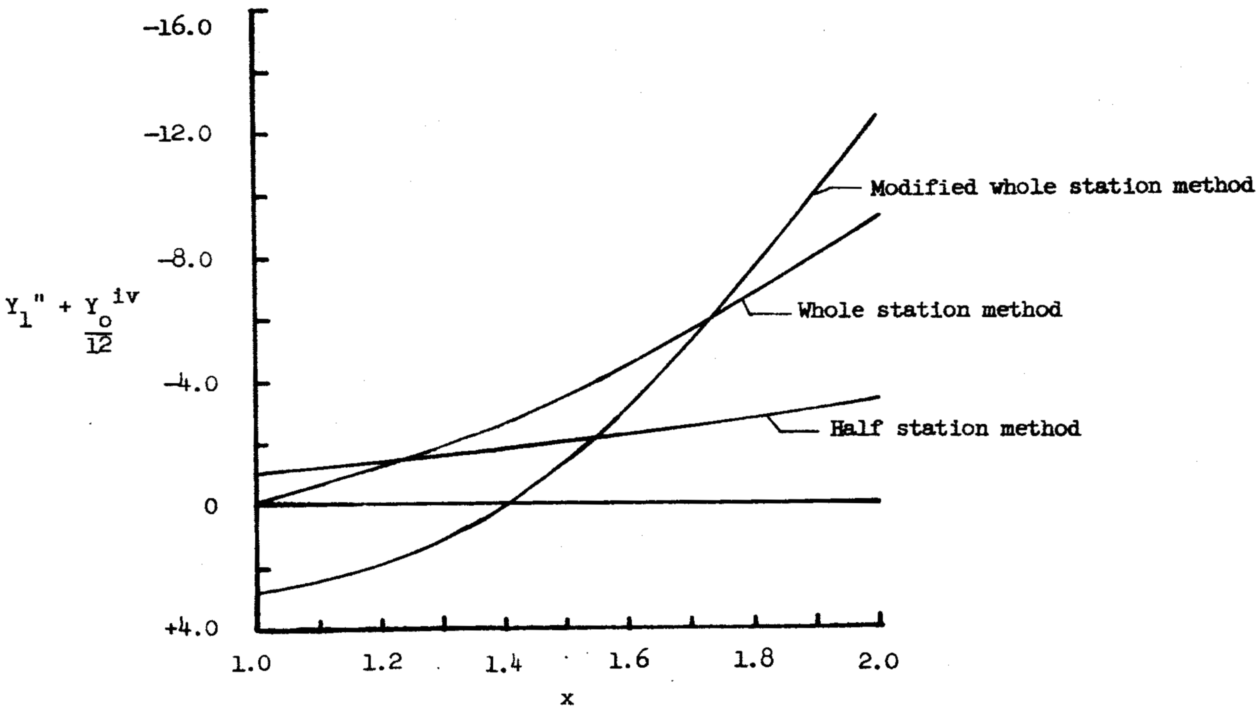
(a) Exact solution.

(b) Error term in approximation solution independent of increment, h.

Figure 2.- $f(x) = 1/x^3$.

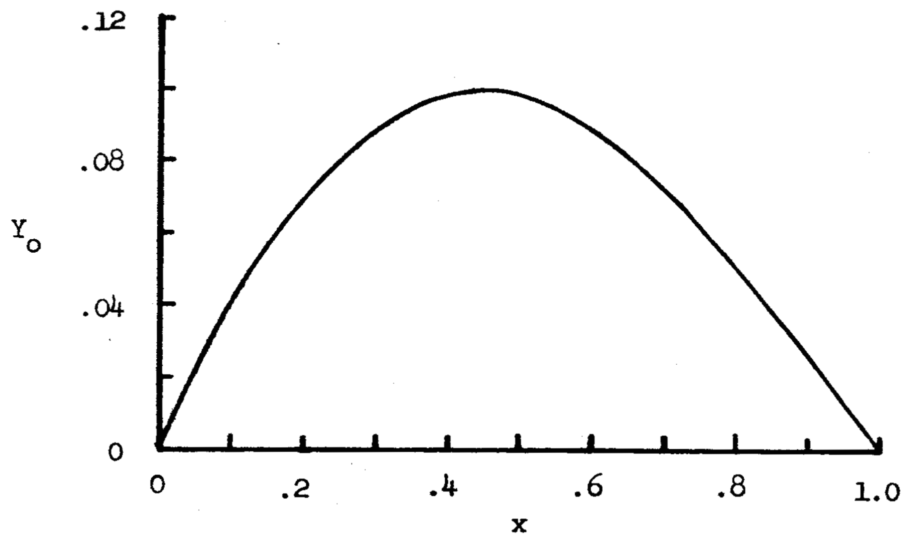


(c) Second derivative of exact solution.

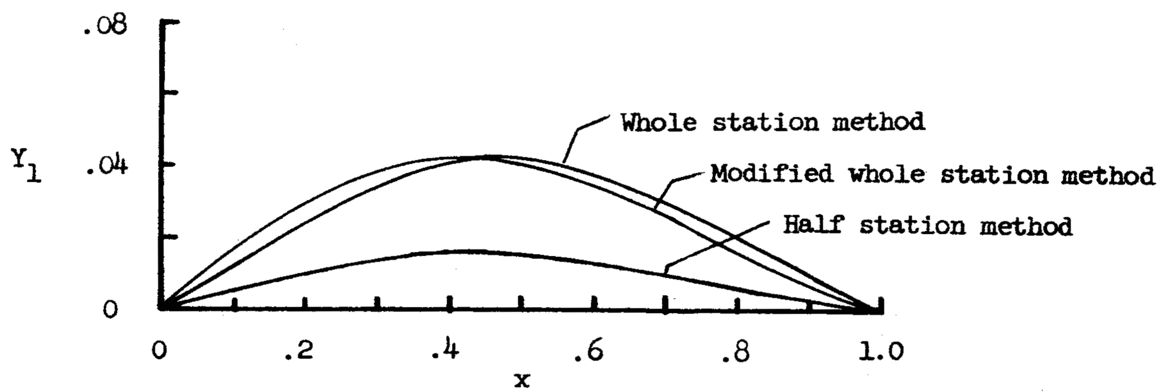


(d) Error term in approximate solution of second derivative independent of increment, h.

Figure 2.- Concluded.

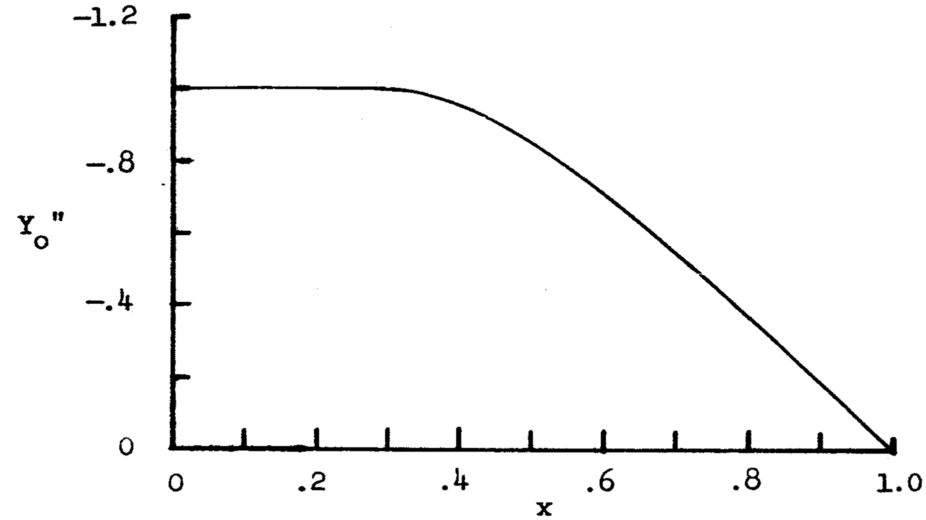


(a) Exact solution.

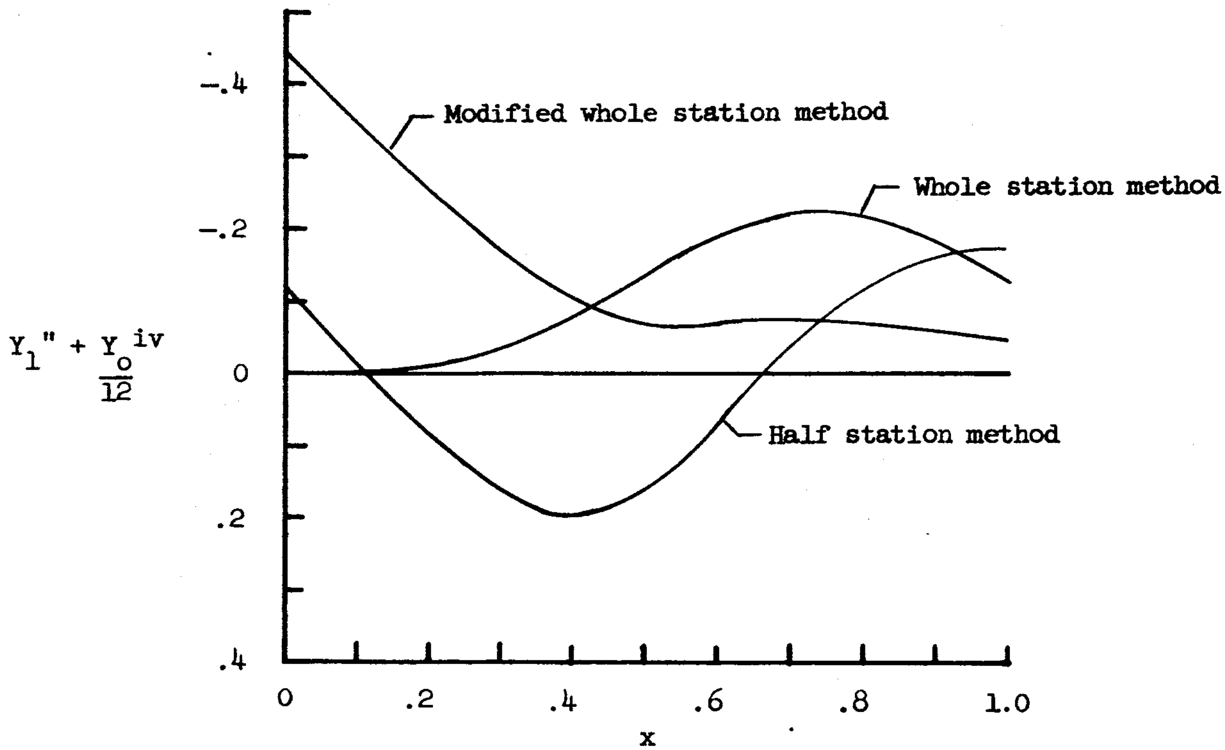


(b) Error term in approximate solution independent of increment, h.

Figure 3.- $f(x) = 1 + x^3$.

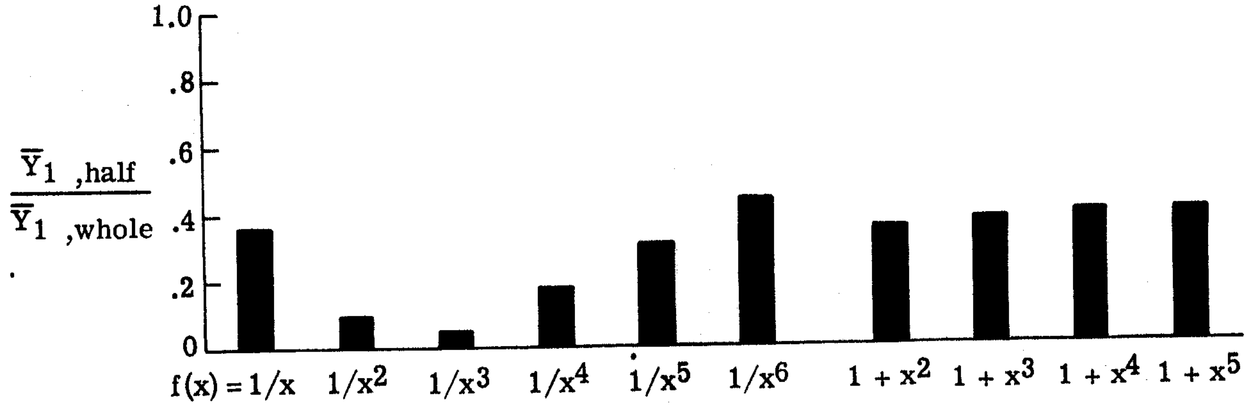


(c) Second derivative of exact solution.

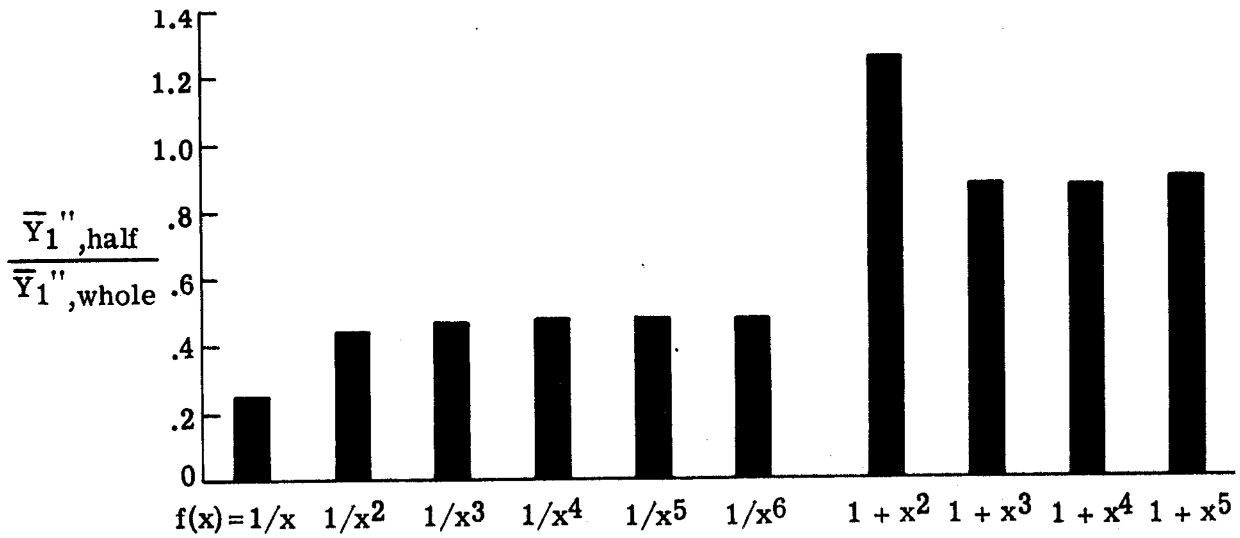


(d) Error term in approximate solution of second derivative independent of increment, h.

Figure 3.- Concluded.

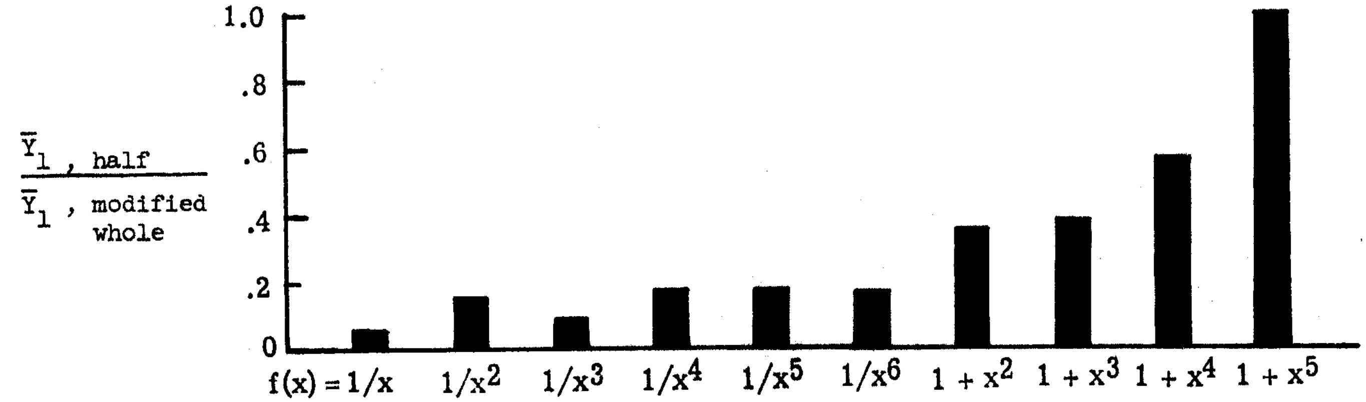


(a) Deflection.

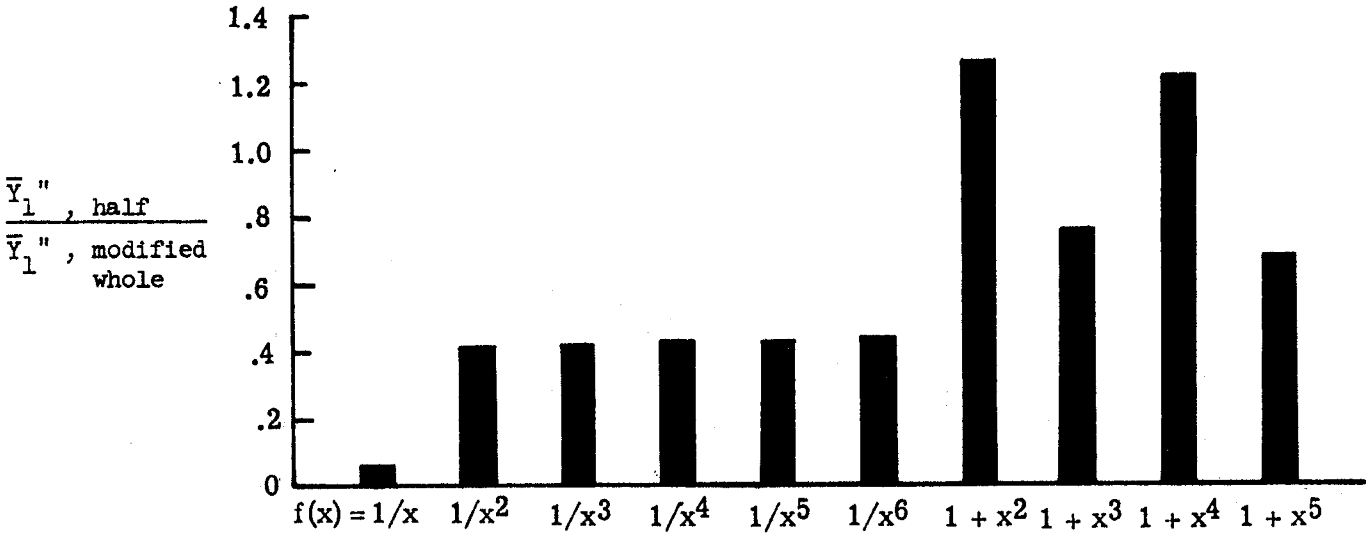


(b) Second derivative.

Figure 4.- Ratio of root mean square errors for half and whole station methods.



(a) Deflection.



(b) Second derivative.

Figure 5.- Ratio of root mean square errors for half and modified whole station methods.